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Anisotropy of the optical conductivity of high T_c cuprates

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(October 4, 2006)

The optical conductivity along (σ_{xx}) and perpendicular (σ_{zz}) to the planes is calculated assuming strong k_{\parallel} -dependence of the scattering rate and the c-axis hopping parameter. The closed analytical expressions for $\sigma_{xx}(\omega)$ and $\sigma_{zz}(\omega)$ are shown to be integrable at low and high frequencies. A large and qualitatively different frequency dependence for both polarizations follows directly from the model. The expression for $\sigma_{xx}(\omega)$ has an effective scattering rate proportional to frequency, and can be easily generalized to provide a simple analytical expression, which may replace the Drude formula in the case of non-Fermi liquids.

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The anomalous transport characteristics in the normal state of the high T_c superconductors^{1,2}, and the corresponding quasi-particle properties in the superconducting state have been discussed in a series of recent papers emphasizing strong anisotropy of quasiparticles as a function of position around the Fermi-surface³⁻⁵. Such anisotropies have been used both in the framework of non-Fermi-liquid models *and* Fermi-liquid motivated models^{6,7}. In the models considered in Refs.^{4,5}, anomalous strong scattering of quasi-particles is assumed in the Fermi surface regions closest to the saddle-points, while weak scattering is assumed in the zone-diagonal directions in k -space along 0 to (π, π) . Stojkovic and Pines⁴ used a frequency and k -dependent self-energy for numerical calculations of the in-plane optical properties and magnetotransport of the cuprates. Ioffe and Millis (I&M)⁵ proposed an analytic expression for the k -dependent self energy, containing *no* explicit frequency dependence. The resulting expression for the optical conductivity corresponds to a Fermi-surface average of Lorentzian response functions with a k -dependent scattering rate. Interestingly this expression may be 'correct' (at least approximately) irrespective whether the underlying model is Fermi-liquid or not. The strong momentum dependence of the scattering rate is experimentally motivated by Angle Resolved Photo Electron Spectra⁸. We will see in this paper, that this model provides an excellent description of both the out-of-plane and in-plane optical properties of high T_c superconductors. We take the expression of Ref.⁵ for the Fermi-surface averaged optical conductivity as our starting point

$$\sigma_{xx}(\omega) = \frac{ne^2}{2\pi m_{xx}} \int_0^{2\pi} d\theta \frac{i}{\omega + i\gamma(\theta)} \quad (1)$$

In this expression θ is the angle along the Fermi surface relative to the (π, π) direction, $n = k_F^2/2\pi d$ is the density of electrons, $m_{xx} = \hbar k_F/v_F$ is the planar effective mass, and d the distance between planes. For $\gamma(\theta)$ isotropic the classical Drude formula is recovered. (Note a factor $1/4\hbar d$ difference with Eq. 13 of Ref.⁵). I&M

furthermore postulated the following formula for the k -dependent scattering rate, motivated by photoemission experiments on a variety of high T_c superconductors

$$\gamma(k_{\parallel}) = 1/\tau + \Gamma \sin^2(2\theta) \quad (2)$$

Inserting this expression for the scattering rate in Eq. 1, substituting $\xi = e^{2i\theta}$, carrying out the corresponding contour integral, and using Cauchy's principle value method, we obtain the planar conductivity

$$\sigma_{xx}(\omega) = \frac{\sigma_{xx,0}}{\sqrt{1 - i\omega\tau}\sqrt{1 + \Gamma\tau - i\omega\tau}} \quad (3)$$

where $\sigma_{xx,0} \equiv ne^2\tau/m_{xx}$. In the approximation of Ref.⁵, valid close to the zone-diagonals, the term $(\omega + i\Gamma)^{1/2}$ is replaced with the constant $(i\Gamma)^{1/2}$, resulting in non-integrable behavior of $\text{Re}\sigma_{xx}(\omega)$ at high frequencies. I&M adopted the model assumption, that $1/\tau$ should have a quadratic temperature dependence, $1/\tau = T^2/T_0$, as in a classical Fermi-liquid. (But note, that *only* the zone-diagonal directions have a scattering rate which becomes zero at low temperature in their model, which is anything but Fermi-liquid behavior). The DC-resistivity then has the linear temperature dependence $\rho = \Gamma^{1/2}T_0^{-1/2}m_{xx}T/(ne^2)$, observed in optimally doped cuprates.

Let us briefly investigate some of the main analytical properties of the above result. First we notice, that $\sigma(\omega) = \sigma(-\omega)^*$ is satisfied. Let us now consider the frequency dependent scattering rate, using the definition $1/\tau^*(\omega) \equiv \omega \text{Re}\sigma/\text{Im}\sigma$, commonly used for the analysis of optical spectra of high T_c superconductors and heavy Fermion systems

$$\frac{1}{\tau^*(\omega)} = \frac{(1 + \Gamma\tau) \sqrt{1 + (\omega\tau)^2} + \sqrt{(1 + \Gamma\tau)^2 + (\omega\tau)^2}}{\tau \left[\sqrt{1 + (\omega\tau)^2} + \sqrt{(1 + \Gamma\tau)^2 + (\omega\tau)^2} \right]} \quad (4)$$

At intermediate frequencies, $1/\tau \ll \omega \ll \Gamma$, the scattering rate $1/\tau^*(\omega) = \omega$. The high frequency limiting behavior of these quantities gives

$$\lim_{\omega \rightarrow \infty} \sigma_{xx}(\omega) = \frac{ne^2}{m_{xx}} \frac{i}{\omega + i(1/\tau + \Gamma/2)} \quad (5)$$

The low frequency limiting behavior corresponds to a Drude conductivity

$$\sigma_D(\omega) = \lim_{\omega \rightarrow 0} \sigma_{xx}(\omega) = \frac{Z^*(0)ne^2}{m_{xx}} \frac{i}{\omega + i/\tau^*(0)} \quad (6)$$

with the scattering rate $\tau^*(0)$ and the spectral weight $Z^*(0)$ defined as

$$\tau^*(0) = \frac{\tau \Gamma \tau + 2}{2 \Gamma \tau + 1} = \frac{T_0}{2T^2} + \frac{1}{2\Gamma} + \dots,$$

$$Z^*(0) = \frac{\int_0^\infty \sigma_D(\omega) d\omega}{\int_0^\infty \sigma_{xx}(\omega) d\omega} = \frac{2}{\sqrt{1 + \Gamma \tau}} = \frac{2T}{\sqrt{\Gamma T_0}} - \frac{T^3}{\{\Gamma T_0\}^{3/2}} + \dots \quad (7)$$

where the series expansion is relevant for at low temperatures, where τ diverges. Taken together, we see that σ_{xx} is integrable, and satisfies

$$\int_0^\infty \text{Re} \sigma_{xx}(\omega) d\omega = \frac{\pi ne^2}{2m_{xx}} \quad (8)$$

We see, that for $T \ll \sqrt{T_0 \Gamma}$, which is of the order of 1000 K, $1/\tau^*(0)$ is proportional to T^2 , and that the low frequency spectral weight $Z^*(0)$ increases linearly with temperature. It is amusing, that, apart from a factor two, the inverse Hall constant derived in Ref.⁵ is precisely this spectral weight: $1/R_H = B\sigma_{xx}^2/\sigma_{xy} = 2eZ^*(0)n$.

In various papers a linear temperature dependence of the scattering rate of the low-frequency Drude tail has been reported. However, a fit to Hagen-Rubens behavior provides the DC conductivity $\sigma_{xx} = Z^*(0)ne^2\tau^*(0)/m_{xx}$. Usually a temperature independent Drude spectral weight is imposed for the purpose of minimizing the number of fit parameters. However, the 'Drude scattering rate' resulting from such a fit, is not a faithful representation of the actual line-width of $\sigma_D(\omega)$ if $Z^*(0) < 1$. Instead one can employ the fact, that $1/\tau^*(\omega) = \omega \text{Re} \sigma_{xx}(\omega) / \text{Im} \sigma_{xx}(\omega)$ and $Z^*(\omega) = \text{Im}[-ne^2/(4m_{xx}\pi\omega\sigma_{xx}(\omega))]$ can be obtained from a careful analysis of the DC limiting behavior of the experimentally measured real and imaginary part of the conductivity. This should reveal both the quadratic temperature dependence of $1/\tau$ and the linear temperature dependence of the low frequency spectral weight. Although this behavior has, to my best knowledge, not been mentioned explicitly in the literature, it may be contained in the experimental infrared data reported by various groups⁹. This aspect certainly requires further scrutiny, and calls for high precision optical experiments in the far infrared range.

In Fig. 1 the evolution of $\sigma_{xx}(\omega)$ with temperature is displayed, mimicked by varying the parameter $1/\tau$. This behavior is identical to what has been observed experimentally for the in-plane optical conductivity^{10,9,11}. Note

also, that the total spectral weight under the optical conductivity curves is the same for all values of $1/\tau$.

Let us now investigate the behavior of σ_{zz} . Recently Xiang and Wheatley³ calculated the c-axis penetration depth assuming d-wave pairing, and assuming a model for the c-axis transport where momentum parallel to the planes, k_{\parallel} , is conserved. Based on LDA band theoretical results¹² they argued, that for HTSC's with a simple (non-body centered) tetragonal structure, $t_{\perp} \propto (\cos(k_x a) - \cos(k_y a))^2$, leading to a T^5 powerlaw at low temperature. Following the approach used in Refs.³⁻⁵ this k -dependence is evaluated as a function of k_{\parallel} around the Fermi surface.

The c-axis conductivity is, in leading orders of t_{\perp} ¹³

$$\sigma_{zz}(\omega) = \frac{e^2 dm_{xx}}{\pi^2 \hbar^4} \int_0^{2\pi} d\theta \frac{t_{\perp}(\theta)^2}{-i\omega + \gamma(\theta)} \quad (9)$$

A simple hole, or electron-type surface is circular, and has the following k_{\parallel} -dependence in leading orders of the harmonic expansion

$$t_{\perp}(k_{\parallel}) = t_0 \sin^2(2\theta) \quad (10)$$

Note, that the expression for σ_{zz} now contains a weighting factor proportional to $\sin^4(2\theta)$, which is sharply peaked along $(0, \pm\pi)$ and $(\pm\pi, 0)$. Again the integral can be solved using Cauchy's principle value method, with the result

$$\frac{\sigma_{zz}(\omega)}{\sigma_{zz,0}} = 1 + 2\Omega^2 \left[\sqrt{\frac{\Omega^2}{1 + \Omega^2}} - 1 \right] \quad (11)$$

where $\Omega \equiv \sqrt{(1 - i\omega\tau)/(\Gamma\tau)}$, and $\sigma_{zz,0} \equiv e^2 dm_{xx} t_0^2 / (\pi \hbar^4 \Gamma)$. I&M needed a value of $\hbar\Gamma$ of about 0.15 eV to fit $\sigma_{xx}(\omega)$ of YBCO¹⁴. In fact, if we use Eq.3 for $\sigma_{xx}(\omega)$, a larger value is required, $\hbar\Gamma \approx 1.2\text{eV}$ to produce a good fit. Both values place the c-axis-transport well inside the dirty limit region, if we adopt Eq. 11 as an expression representative of the c-axis optical conductivity in the normal state of high T_c superconductors.

The analytical formula for $1/\tau^*(\omega)$ according to Eq. 11 is a rather lengthy expression, which is not very illuminating. To obtain further insight in the effect of a strongly anisotropic scattering rate around the Fermi surface on the optical properties, in Fig. 2 both σ_{xx} and σ_{zz} and the corresponding frequency dependent scattering rates are presented, adopting $\hbar/\tau = 12.4\text{meV}$, and $\hbar\Gamma = 1.24\text{eV}$ as model parameters. Clearly σ_{zz} is dominated by the transport in the regions close to the saddlepoints, resulting in a frequency dependent scattering rate ranging from about $\Gamma/2$ at low frequencies, to Γ at high frequencies. The calculated spectral shape resembles closely the experimental data^{16,15,17-23}.

At this point it should be noted however, that the model assumption for the k_{\parallel} -dependence of t_{\perp} is only justified for cuprates with the simple tetragonal structure, in particular Hg1201 or Tl1201. Materials like LSCO, Tl2201,

and Bi2212, which have been studied more intensively during recent years, have a body centered tetragonal structure, for which

$$t_{\perp} \propto (\cos(k_x a) - \cos(k_y a))^2 \cos(k_x a/2) \cos(k_y a/2) \quad (12)$$

Hole-type Fermi-surfaces cross not only the zone-diagonal directions, but also the lines $k_x = \pi$ and $k_y = \pi$, where extra zeros occur. The integration over θ in Eq. 9 thus contains eight zero's, along the $(0, \pm\pi)$, $(\pm\pi, 0)$, and $(\pm\pi, \pm\pi)$ directions. The lowest order harmonic expansion of the angular dependence in this case is

$$t_{\perp}(k_{\parallel}) = t_0 \sin^2(4\theta) \quad (13)$$

resulting in the following expression for the c-axis optical conductivity

$$\frac{\sigma_{zz}(\omega)}{2\sigma_{zz,0}} = (1 + 2\Omega^2)(1 - 8\Omega^4 - 8\Omega^2) + 16\Omega^3(1 + \Omega^2)^{3/2} \quad (14)$$

The real part of this expression, and the corresponding $1/\tau^*(\omega)$ are displayed in Fig. 2, using the same parameters as before. We observe from this Figure, that for the body centered systems $\sigma_{zz}(\omega)$ is somewhat more peaked. This results from the fact that contributions from the regions close to the saddle points are suppressed in this case.

Eq. 1 for σ_{xx} , suggests a form which is of general use in other materials (not necessarily 2-dimensional) to analyze the optical conductivity of non-Fermi liquids with a simple analytical formula

$$\sigma_A(\omega) = \frac{\omega_p^2}{4\pi} \frac{i}{(\omega + i/\tau)^{1-2\alpha}(\omega + i\Gamma)^{2\alpha}} \quad (15)$$

If we set $\tau \rightarrow \infty$, and consider only $\omega \ll \Gamma$, this corresponds to the expression derived by Anderson² based on the Luttinger liquid model for high T_c superconductors. The notation for the coefficient α was adopted accordingly. In Anderson's paper Fermi-liquid response is restored for $\alpha \rightarrow 0$, as in the present case. Let us briefly investigate some of the main analytical properties of σ_A . Again $\sigma_A(\omega) = \sigma_A(-\omega)^*$ is satisfied. The high frequency limiting behavior of σ_A

$$\lim_{\omega \rightarrow \infty} \sigma_A(\omega) = \frac{\omega_p^2}{4\pi} \frac{1}{(1 - 2\alpha)/\tau + 2\alpha\Gamma - i\omega} \quad (16)$$

guarantees, that σ_A is integrable, and satisfies

$$\int_0^{\infty} \text{Re}\sigma_A(\omega) d\omega = \frac{1}{8} \omega_p^2 \quad (17)$$

At the low frequency end

$$\lim_{\omega \rightarrow 0} \sigma_A(\omega) = \frac{\omega_p^2}{4\pi} \frac{\tau^{(1-2\alpha)}\Gamma^{-2\alpha}}{1 - i\omega[(1 - 2\alpha)\tau + 2\alpha/\Gamma]} \quad (18)$$

which corresponds to a narrow Drude peak with an effective carrier life-time $\tau^*(0) = (1 - 2\alpha)\tau + 2\alpha/\Gamma$. The frequency dependent scattering rate $1/\tau^*(\omega)$ crosses over to a linear frequency dependence for $1/\tau \ll \omega \ll \Gamma$, and acquires a constant value $(1 - 2\alpha)/\tau + 2\alpha/\Gamma$ for $\omega \rightarrow \infty$. Hence the linear frequency dependence of the scattering rate is a robust property of the above phenomenological expression for σ_A . To illustrate this point, in Fig. 3 $\sigma_A(\omega)$, the corresponding $1/\tau^*(\omega)$ and $1/Z^*(\omega)$ are displayed for a number of different values of α . The Luttinger liquid analysis of experimental spectra^{2,26} gave $\alpha = 0.15 \pm 0.05$. The analysis of Ioffe and Millis corresponds to $\alpha = 0.25$, which is reasonably close.

In conclusion, the combination of the k-dependent scattering rate, and the k-dependence of the inter-plane hopping parameter known from band theory, leads to a quantitative description of the strongly anisotropic optical properties found in the high T_c cuprates. Both the anomalous in-plane optical conductivity and the c-axis conductivity follow from the assumption of the k-dependent scattering rate, which has been recently proposed by Stojkovich, Pines⁴, Ioffe and Millis⁵. Closed analytical expressions were obtained for the optical conductivity, which are really quite simple, and were further extended and discussed in a phenomenological framework of non-Fermi liquids. The present result corresponds closely to experimental data of $\sigma_{xx}(\omega)$ ^{14,24-26}, including the high frequency cutoff and the low frequency cross-over to Drude behavior as can be seen from the saturation, and of $\sigma_{zz}(\omega)$ ^{15,17-20}.

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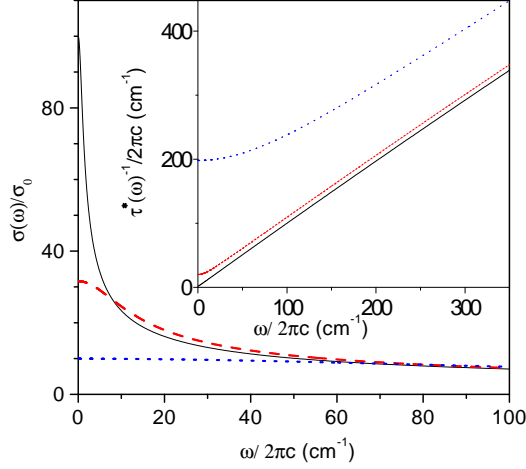


FIG. 1. Optical conductivity, σ_{xx} , using Eq. 3, with parameters $\hbar\Gamma = 1.24\text{eV}$ and $\hbar/\tau = 0.124\text{meV}$ (solid curves, $T = 14\text{ K}$), $\hbar/\tau = 1.24\text{meV}$ (dashed curves, $T = 44\text{ K}$), $\hbar/\tau = 12.4\text{meV}$ (dotted curves, $T = 140\text{ K}$). The temperatures correspond to $1/\tau = T^2/T_0$, adopting the value $T_0 = 12\text{meV}$ from Ioffe and Millis. Inset: Frequency dependent scattering corresponding to the conductivities displayed in the main panel.

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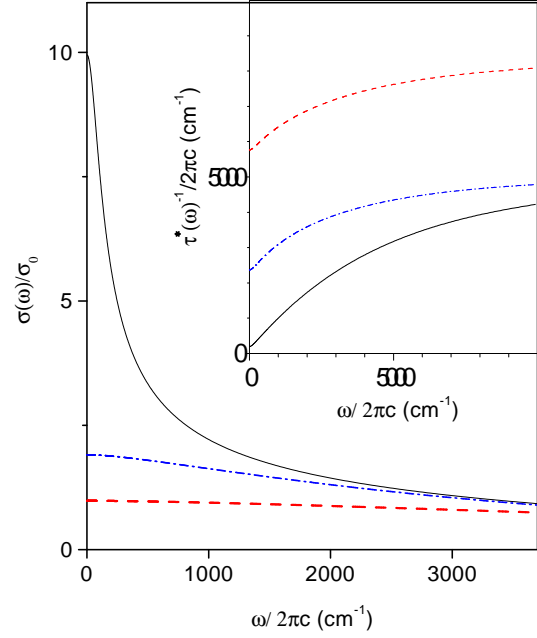


FIG. 2. Optical conductivity using the parameters $\hbar/\tau = 12.4\text{meV}$ and $\hbar\Gamma = 1.24\text{eV}$. Solid curves σ_{xx} , using Eq. 3. Dashed: σ_{zz} for the simple tetragonal structure using Eq. 11. Dashed-dotted: σ_{zz} for the body centered tetragonal structure using Eq. 14. Inset: Frequency dependent scattering corresponding to the conductivities displayed in the main panel.

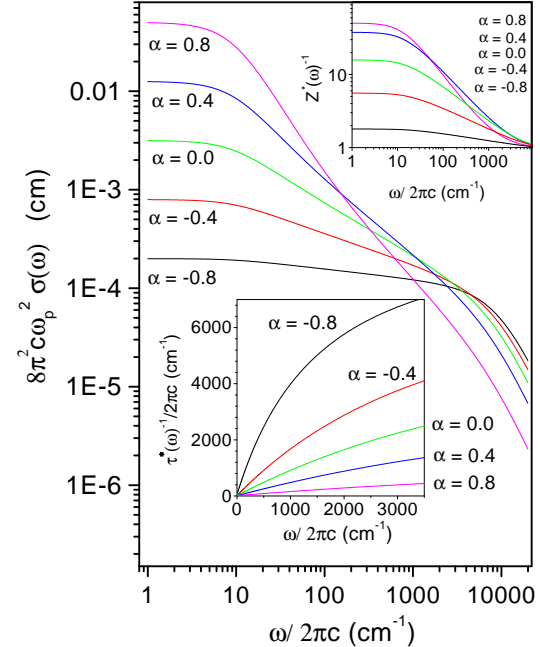


FIG. 3. Optical conductivity using Eq. 15, with the parameters $\hbar/\tau = 1.24\text{meV}$ and $\hbar\Gamma = 1.24\text{eV}$, and $\alpha = 0.8, 0.4, 0.0, -0.4$, and -0.8 . Insets: Frequency dependent scattering rate and spectral weight factor.